

# Diethyl p-aminobenzylphosphonate

**Other names:**

Diethyl 4-aminobenzylphosphonate  
4-Amino benzyl diethyl phosphonate  
Phosphonic acid, [(4-aminophenyl)methyl]-, diethyl ester  
p-Aminobenzylphosphonic acid diethyl ester  
Phosphonic acid, p-aminobenzyl-, diethyl ester

**Inchi:**

InChI=1S/C11H18NO3P/c1-3-14-16(13,15-4-2)9-10-5-7-11(12)8-6-10/h5-8H,3-4,9,12H2,

**InchiKey:**

ZVAYUUUQOCPZCZ-UHFFFAOYSA-N

**Formula:**

C<sub>11</sub>H<sub>18</sub>NO<sub>3</sub>P

**SMILES:**

CCOP(=O)(Cc1ccc(N)cc1)OCC

**Mol. weight [g/mol]:**

243.24

**CAS:**

20074-79-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.035		Crippen Method
mcvol	190.140	ml/mol	McGowan Method

## Sources

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C20074797&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:**

Log10 of Water solubility in mol/l

**logp:**

Octanol/Water partition coefficient

**mcvol:**

McGowan's characteristic volume

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